IL 12

Recent investigations on O(^1D)+D_2 and C(^1D)+H_2 reactions and isotopic variants

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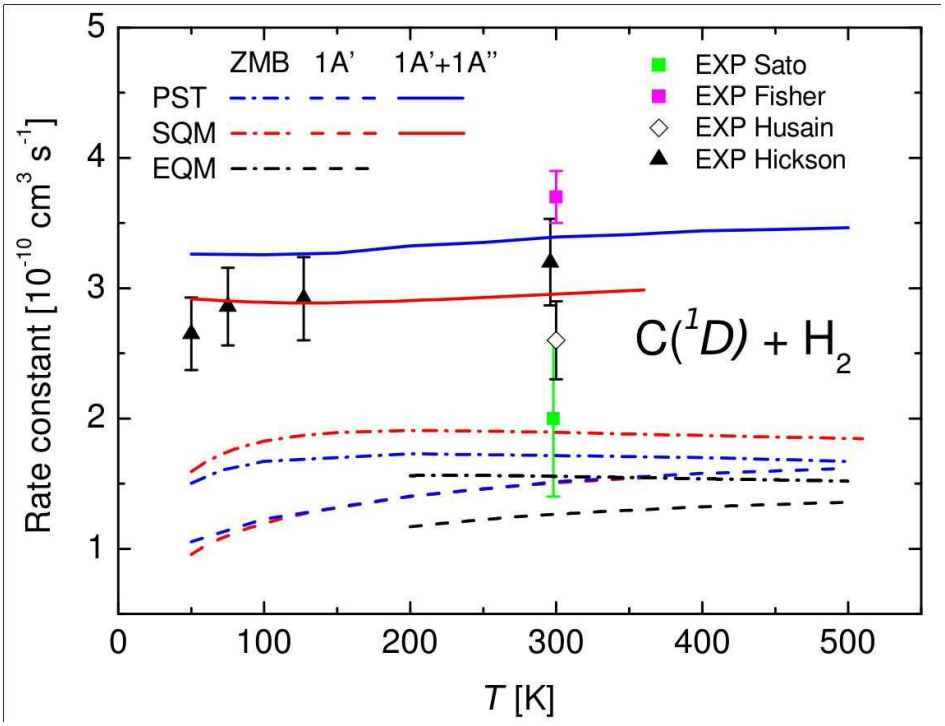
We have carried out theoretical calculations to study the dynamics of X+H_2, where X = O(^1D) or C(^1D), reactions and isotopic variants where hydrogen atoms are substituted by deuterium at low temperature by means of a statistical quantum method [1]. Integral cross sections at the low energy regime and rate constants [2, 3] have been obtained and compared with results obtained by means of exact quantum mechanical approaches and phase space theory. In addition to this, recent experimental investigations on these processes constituted a useful benchmark to test both the theoretical predictions and the role played by different electronic potential energy surfaces.



References

[1] T. González-Lezana, *Int. Rev. Phys. Chem*. **26**, 26-91 (2007)
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